1,3-Propanediol, ethyl octadecyl ether

Inchi: InChI=1S/C23H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-25-23-20-22-24-4-2

InchiKey: KGITULWCVXOERK-UHFFFAOYSA-N

Formula: C23H48O2

SMILES: CCCCCCCCCCCCCCCCCCCOCCCOCC

Mol. weight [g/mol]: 356.63

Physical Properties

Property code	Value	Unit	Source
gf	-67.22	kJ/mol	Joback Method
hf	-782.49	kJ/mol	Joback Method
hfus	57.70	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	7.691		Crippen Method
mcvol	346.670	ml/mol	McGowan Method
pc	835.31	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	770.48	K	Joback Method
tc	943.94	K	Joback Method
tf	393.43	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.14	J/mol×K	770.48	Joback Method
cpg	1195.52	J/mol×K	915.03	Joback Method
cpg	1177.49	J/mol×K	886.12	Joback Method
cpg	1158.46	J/mol×K	857.21	Joback Method
cpg	1138.40	J/mol×K	828.30	Joback Method
cpg	1117.31	J/mol×K	799.39	Joback Method
cpg	1212.57	J/mol×K	943.94	Joback Method
dvisc	0.0000378	Pa×s	770.48	Joback Method

dvisc	0.0000517	Pa×s	707.64	Joback Method
dvisc	0.0000752	Pa×s	644.80	Joback Method
dvisc	0.0001186	Pa×s	581.96	Joback Method
dvisc	0.0002088	Pa×s	519.11	Joback Method
dvisc	0.0004298	Pa×s	456.27	Joback Method
dvisc	0.0011138	Pa×s	393.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406354&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume